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THE OPTICAL SCHRÖDINGER EQUATION[1]

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Paraxial light wave and matter wave optics are compared. Within the paraxial approximation the slowly varying amplitude of a light field in a dielectric medium with a spatially dependent refractive index satisfies an equation which has the form of a Schrödinger equation: the 'optical Schrödinger equation'. The customary procedure of neglecting second order derivatives is replaced by a systematic expansion which allows the calculation of corrections to the lowest order result. The general theory is illustrated in an example.

1. Introduction

The investigation of paraxial wave propagation is certainly not a new topic; numerous authors have studied paraxial optics for light waves [1]-[3] and for matter waves [4],[5]. The emphasis of the present work, however, lies on the direct comparison of the two phenomena, which has also been adressed by Bordé [6]. Furthermore, there are new experimental developments which make such questions interesting again from new perspectives: fiber optics on the optical side and trapping and cooling of neutral atoms and atom interferometry on the mater wave side.

The evolution of a massive quantum particle and a travelling light pulse are both wave phenomena and thus have many similarities; for instance the time-independent Schrödinger equation of quantum mechanics resembles the Helmholtz equation of classical electrodynamics. Apart from the probabilistic interpretation of the quantum wavefunctions, an important distinction between a light pulse and a Schrödinger particle is the vacuum dispersion relation: as a consequence of their quadratic dispersion relation, matter waves cannot retain the shape of their wavepackets as they propagate through

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empty space, since the group velocity and the phase velocity differ – in contrast to light waves in vacuum.

However, in an inhomogeneous transparent medium, the similarities in the propagation of matter waves and light waves can be particularly close, because the dispersion relation of light waves in the medium differs from the linear vacuum dispersion relation. If one makes the paraxial approximation in this case, one obtains an equation which is formally a Schrödinger equation [6],[7]. In this paper we will make a quantitative comparison between a paraxial (quasi)monochromatic light beam propagating in such a dielectric medium and its Schrödinger analogue. Our goal is to estimate the 'optical corrections' to the Schrödinger equation. In this paper, for the sake of simplicity, we will concentrate on scalar fields, but our approach is also applicable to true vector field situations, as will be discussed elsewhere.

2. The paraxial approximation

We consider a paraxial and quasimonochromatic wavepacket with main propagation direction along the z-direction, i.e. $\mathbf{k} \approx \mathbf{k}_0 = k_0\mathbf{e}_z$ and $\omega \approx \omega_0 = ck_0$ propagating in an inhomogeneous dielectric medium with an electric susceptibility $\epsilon(\mathbf{x}) \equiv \epsilon(\omega \approx \omega_0; \mathbf{x})$ and thus a spatially dependent refractive index $\epsilon(\mathbf{x}) = n^2(\mathbf{x})$. For some types of polarization the three vector components of the electric field decouple and one can use a scalar wave equation [8].

Let our starting point thus be the scalar wave equation

$$\frac{n^2(\mathbf{x})}{c^2}\frac{\partial^2}{\partial t^2} E(\mathbf{x},t) = \nabla^2 E(\mathbf{x},t) . \tag{1}$$

Splitting the field amplitude $E(\mathbf{x},t)$ into a rapidly and a slowly varying factor

$$E(\mathbf{x},t) = \alpha_0\, e^{i\varphi(\mathbf{x})-i\omega_0 t}\, \mathcal{E}(\mathbf{x},t) ; \tag{2}$$

with some suitably chosen phase factor $\varphi(\mathbf{x})$, the slowly varying amplitude $\mathcal{E}(\mathbf{x},t)$ satisfies the equation

$$\frac{n^2(\mathbf{x})}{c^2}\left(\frac{\partial}{\partial t} - i\omega_0\right)^2 \mathcal{E}(\mathbf{x},t) = \nabla_\varphi^2 \mathcal{E}(\mathbf{x},t) , \tag{3}$$

where we have defined $\nabla_\varphi = \nabla + i(\nabla\varphi)$.

The paraxial and quasimonochromatic approximations correspond to neglecting the $\partial^2/\partial z^2$ and $\partial^2/\partial t^2$ derivatives of the slowly varying amplitude, on grounds that

$$\left|\frac{\partial^2\mathcal{E}}{\partial z^2}\right| \ll k_0 \left|\frac{\partial\mathcal{E}}{\partial z}\right| , \qquad \left|\frac{\partial^2\mathcal{E}}{\partial t^2}\right| \ll \omega_0 \left|\frac{\partial\mathcal{E}}{\partial t}\right| . \tag{4}$$

For monochromatic fields with time-independent slowly varying amplitude $\mathcal{E}(\mathbf{x},t) = \mathcal{E}(\mathbf{x})$ and setting $\varphi(\mathbf{x}) = k_0 n_0 z$ (with n_0 being some typical value of the refractive index) this procedure leads to

$$i\frac{\partial}{\partial \tau}\psi(x,y;\tau) = -\frac{1}{2k_0^2 n_0^2}\nabla_\perp^2\psi(x,y;\tau) - \frac{1}{2}\left[\frac{n^2(\mathbf{x}) - n_0^2}{n_0^2}\right]\psi(x,y;\tau) \tag{5}$$

with $\psi(x,y;\tau = k_0 n_0 z) = \mathcal{E}_i(\mathbf{x})$ for $i \in \{x,y,z\}$ and the definition $\nabla_\perp^2 \equiv (\partial^2/\partial x^2 + \partial^2/\partial y^2)$. This equation is formally a Schrödinger equation for a fictitious particle of 'mass' $m = (k_0 n_0)^2$ evolving in the potential $V_{opt}(\mathbf{x}) = (n^2(\mathbf{x}) - n_0^2)/2n_0^2$ in a (dimensionless) time $\tau = k_0 n_0 z$ [7]. Thus the 3D Hel mholtz equation is approximated by a Schrödinger equation with a two-dimensional potential, which is in general also 'time'-dependent. Note that the 'optical potential' in this context must *necessarily* be a small perturbation (i.e. $n^2(\mathbf{x}) \approx n_0^2$) for condition Eq.(4) and the separation into a 'slowly' and a 'rapidly' varying part to be reasonable.

If one is interested in a quantitative comparison of paraxial wave propagation of ligth and matter waves and wants to calculate the non-paraxial 'optical corrections' to the Schrödinger solution, a more systematic approach is required. Like Lax et al. [2], who investigated the paraxial approximation for wave propagation in a medium with nonlinear refractive index, and by Garrison and Deutsch [4] for paraxial wave propagation of quantum particles in free space, we introduce a sma ll expansion parameter: the angle Θ between the $\mathbf{k}$-vectors in the propagating beam and the wave-vector $\mathbf{k}_0 = k_0\mathbf{e}_z$ of the 'carrier' plane wave propagating in z-direction. Defining

$$\Theta = \angle(\mathbf{k}_0, \mathbf{k}), \qquad \mathbf{k} = \mathbf{k}_0 + \mathbf{q} \tag{6}$$

it follows from a simple geometric argument that the transverse deviations of the wave-vector scale as $|\mathbf{q}_T|/k_0 = \mathcal{O}(\Theta)$ and *longitudinal* ones as $|q_z|/k_0 = \mathcal{O}(\Theta^2)$. For quasi-monochromatic beams $(\omega - \omega_0)/\omega_0 = \mathcal{O}(\Theta^2)$.

For the series expansion in Θ we rewrite Eq.(3) by formally taking the square root

$$\frac{n(\mathbf{x})}{c}\left(\frac{\partial}{\partial t} - i\omega_0\right)\psi(\mathbf{x},t) = i\sqrt{\nabla_\varphi^2}\,\psi(\mathbf{x},t) , \tag{7}$$

and transform to scaled variables as follows

$$\bar{\mathbf{x}}_T = \Theta k_0 n_0\, \mathbf{x}_T, \quad \bar{z} = \Theta^2 k_0 n_0\, z \equiv \Theta^2\,\tau, \quad \bar{t} = \Theta^2\omega_0\, t . \tag{8}$$

We arrive at

$$i\frac{\partial}{\partial \bar{t}}\psi(\bar{\mathbf{x}},\bar{t}) = \frac{1}{\Theta^2}\left[\frac{1}{n(\bar{\mathbf{x}})}\sqrt{\Theta^4\Delta_4 + \Theta^2\Delta_2 + \Delta_0 + \Theta^{-2}\Delta_{-2}} - 1\right]\psi(\bar{\mathbf{x}},\bar{t}) \tag{9}$$

with

$$\begin{aligned}
\Delta_4 &= -\frac{\partial^2}{\partial \bar{z}^2}\\
\Delta_2 &= -\bar{\nabla}_T^2 - i\frac{\partial\Gamma_{\bar{z}}}{\partial\bar{z}} - 2i\Gamma_{\bar{z}}\frac{\partial}{\partial\bar{z}}\\
\Delta_0 &= \Gamma_{\bar{z}}^2 - i\left(\frac{\partial\Gamma_{\bar{x}}}{\partial\bar{x}} + \frac{\partial\Gamma_{\bar{y}}}{\partial\bar{y}}\right) - 2i\left(\Gamma_{\bar{x}}\frac{\partial}{\partial\bar{x}} + \Gamma_{\bar{y}}\frac{\partial}{\partial\bar{y}}\right)\\
\Delta_{-2} &= \Gamma_{\bar{x}}^2 + \Gamma_{\bar{y}}^2 ,
\end{aligned} \tag{10}$$

and $\Gamma_{\bar{x}_i} = \frac{\partial}{\partial\bar{x}_i}\left[\Theta^2\varphi(\bar{\mathbf{x}})\right] = \mathcal{O}(1)$ with $\bar{x}_i \in \{\bar{x},\bar{y},\bar{z}\}$. So far Eq.(9) is still exact for scalar fields and arbitrary $\varphi(\mathbf{x})$.

We now pull out a 'carrier' plane wave for the expansion in Θ, that is we choose $\varphi(\mathbf{x}) = k_0 n_0 z = \bar{z}/\Theta^2$, which clearly gives rise to fast oscillations for $\bar{z} \sim 1$. The term Δ_{-2}, which is inver sely proportional to Θ, vanishes, since $\Gamma_{\bar{x}}^2 = \Gamma_{\bar{y}}^2 = 0$, and $\Gamma_{\bar{z}}^2 = 1$. For the remaining part of the amplitude to be slowly varying we require

$$k_0 \left[n(\mathbf{x}) - n_0\right] z \equiv \frac{1}{\Theta^2} \left[\bar{n}(\bar{\mathbf{x}}) - n_0\right] \bar{z} \lesssim 1 \quad (11)$$

on the same scale and the deviation from a typical value of the refractive index n_0 is assumed to scale like $\left[n^2(\mathbf{x}) - n_0^2\right]/n_0^2 = \mathcal{O}(\Theta^2)$.

Let us now demonstrate the usefulnes of the series expansion for the special case of *monochromatic* fields (that is ψ is independent of t or the corresponding scaled variable $\bar{t}$), and secondly of refractive indices which has only variations in the *transverse* profile ($n(\mathbf{x}) = n(x, y)$). Expanding the square root in Eq.(9) to lowest order immediately brings us back to the 'optical Schrödinger equation' Eq.(5). For the higher order corrections we expand the 'wavefunction' $\bar{\psi}(\bar{x}, \bar{y}, \bar{z})$ (in scaled variables) in a power series of Θ

$$\bar{\psi}(\bar{x}, \bar{y}; \bar{z}) = \sum_{\mu=0}^{\infty} \Theta^{2\mu}\, \bar{\psi}^{(2\mu)}(\bar{x}, \bar{y}; \bar{z}) \,. \quad (12)$$

Insertion into the wave equation immediately leads to

$$\left[i\frac{\partial}{\partial \bar{z}} - H_T\right] \bar{\psi}^{(0)}(\bar{x}, \bar{y}; \bar{z}) = 0 \qquad \mu = 0 \quad (13)$$

$$\left[i\frac{\partial}{\partial \bar{z}} - H_T\right] \bar{\psi}^{(2\mu)}(\bar{x}, \bar{y}; \bar{z}) = -\frac{1}{2}\frac{\partial^2}{\partial \bar{z}^2}\, \bar{\psi}^{(2\mu-2)}(\bar{x}, \bar{y}; \bar{z}) \qquad \mu = 1, 2, 3, \ldots \quad (14)$$

with

$$\begin{aligned} H_T &= -\bar{\nabla}_T^2 + V_{opt}(\bar{x}, \bar{y}) \\ V_{opt}(\bar{x}, \bar{y}) &= \frac{1}{2}\frac{\left[n_0^2 - \bar{n}^2(\bar{\mathbf{x}})\right]}{n_0^2} \,. \end{aligned} \quad (15)$$

We see that only the lowest order amplitude $\bar{\psi}^{(0)}(\bar{x}, \bar{y}; \bar{z})$ satisfies a Schrödinger equation, the higher order 'optical corrections' are determined by the inhomogeneous equations Eqs.(14).

This hierarchy of equations is solved in the following way: first we determine the eigenbasis $\{\bar{\varphi}_n(\bar{x}, \bar{y})\}$ of H_T and expand the zero-order amplitude $\bar{\psi}^{(0)}(\bar{x}, \bar{y}; \bar{z})$ in this basis with 'time'-independent coefficients $c_n^{(0)}$; since H_T is independent of $\bar{z}$, it commutes with $\partial^2/\partial\bar{z}^2$, which means that the right hand side of Eq.(14) also represents a solution of the homogeneous equation Eq.(13). Setting

$$\bar{\psi}^{(2\mu)}(\bar{x}, \bar{y}; \bar{z}) = \sum_n c_n^{(2\mu)}(\bar{z})\, e^{-i\bar{E}_n \bar{z}} \bar{\varphi}_n(\bar{x}, \bar{y}) \qquad \mu \neq 0 \quad (16)$$

with $\bar{z}$-dependent coefficients, we get the recursion relation

$$\dot{c}_n^{(2\mu)}(\bar{z}) = \frac{i}{2}\, \ddot{c}_n^{(2\mu-2)}(\bar{z}) + \bar{E}_n\, \dot{c}_n^{(2\mu-2)}(\bar{z}) - \frac{i}{2}\, \bar{E}_n^2\, c_n^{(2\mu-2)}(\bar{z}) \,, \quad (17)$$

where the dots represent differentiation with respect to $\bar{z}$. This can easily be solved by iteration, assuming the 'initial condition' $c_n^{(2\mu)}(\bar{z} = 0) = 0$ for $\mu > 0$; the first few optical corrections $C^{(2\mu)}(\bar{z}) \equiv c_n^{(2)}(\bar{z})/c_n^{(0)}$ as functions of $\alpha(\bar{z}) \equiv -\frac{i}{2}\bar{z}\bar{E}_n^2$ are found to be

$$\mu = 1: \quad C^{(2)}(\bar{z}) = \alpha(\bar{z}) \quad (18)$$

$$\mu = 2: \quad C^{(4)}(\bar{z}) = \alpha(\bar{z})\, \bar{E}_n + \frac{\alpha(\bar{z})^2}{2!} \quad (19)$$

$$\mu = 3: \quad C^{(6)}(\bar{z}) = \alpha(\bar{z})\, \frac{5}{4}\bar{E}_n^2 + \frac{\alpha(\bar{z})^2}{2!}\, 2\bar{E}_n + \frac{\alpha(\bar{z})^3}{3!} \quad (20)$$

$$\mu = 4: \quad C^{(8)}(\bar{z}) = \alpha(\bar{z})\, \frac{7}{4}\bar{E}_n^3 + \frac{\alpha(\bar{z})^2}{2!}\, \frac{7}{2}\bar{E}_n^2 + \frac{\alpha(\bar{z})^3}{3!}\, 3\bar{E}_n + \frac{\alpha(\bar{z})^4}{4!} \,. \quad (21)$$

Returning to unscaled variables

$$\psi(x, y; \tau) = \sum_n c_n^{(0)}\, e^{-iE_n\tau}\, \varphi_n(x, y) + \sum_n c_n^{(0)}\left(-\frac{i}{2}\right) E_n^2 \tau\, e^{-iE_n\tau}\, \varphi_n(x, y) + \ldots \,, \quad (22)$$

gives us a rough estimate of the timescale τ_c on which the corrections become important: the first order correction grows linearly with time, and thus the validity of the first order approximation is limited to $\tau \ll \tau_c$ with $\tau_c = 2/E_{n_0}^2$, where E_{n_0} is the eigenvalue belonging to the eigenfunction of maximum overlap with the initial wavefunction. For $\tau \sim \tau_c$ the approximation of the whole sum by the first (few) leading terms breaks down.

4. Harmonic Motion as an Example

One of the simplest possible examples is harmonic motion: we assume that the refractive index is a function of the transverse coordinate x alone, given by $n^2(\mathbf{x}) = n_0^2\,(1 - \kappa^2 x^2)$; in the paraxial approximation (zeroth order) this leads to an optical Schrödinger equation with a h armonic potential

$$V_{opt}(x) = \frac{1}{2}\kappa^2 x^2 \quad (23)$$

corresonding to an angular frequeny $\omega_{HO} = \kappa/k_0 n_0$. (Obviously there is a restriction on the 'coupling strength' q, since $n^2(\mathbf{x})$ has to stay close to n_0^2, i.e. $\kappa^2 x^2 \ll 1$, over the range of x of interest.)

In Fig.1 the 'Helmholtz' and the 'Schrödinger' evolution of the (same) initial Gaussian wavepacket are compared: for the light wave the τ-axis corresponds to the propagation direction z of the wavepacket in the confining refractive index profile, for the corresponding fictitious Schrödinger particle $\tau = k_0 n_0 z$ has the meaning of the (dimensionless) interaction time in the harmonic well; on the left hand side the position distribution $F_S(x; \tau) = |\psi(x; \tau)|^2$ is illustrated by means of a contour plot and compared with the solution $F_H(x, z) = |\mathcal{E}(x, z)|^2$ of the Helmholtz equation on the right

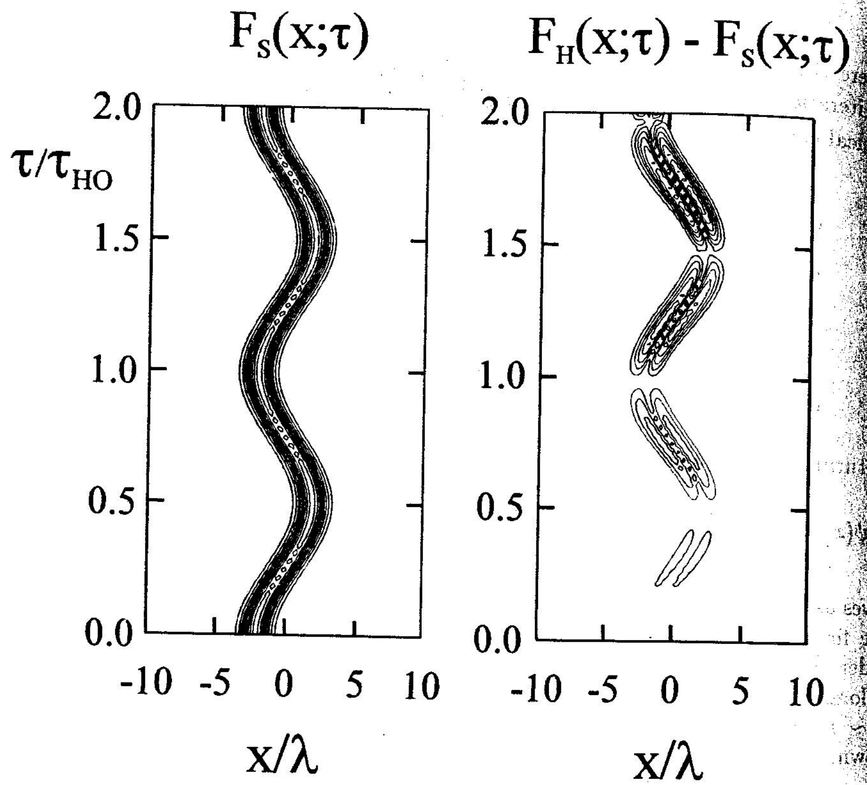

Fig.1. Position distribution of the Schrödinger wavepacket in the harmonic potential (left) and deviations from the full Helmholtz solution (right) for an initial Gaussian wavepacket with $x_0 = -2$ and $\Delta x_0 = \Delta x_{coh}$.

hand side. We have assumed $n_0 = 2$ and $\kappa^2 = 8 \times 10^{-3}/\lambda^2$ with $\lambda = 2\pi/k_0$ being the wavelength of the carrier wave in vacuum, which serves us as typical length scale of the problem. The 'interaction time' τ increases to twice the harmonic oscillation time $t_{HO} = 2\pi/\omega_{HO}$.

We have chosen an initial Gaussian wavepacket with its width Δx_0 being equal to the width $\Delta x_{coh} = 1/\sqrt{2k_0 n_0 \kappa}$ of the ground state in the harmonic potential (coherent state) and an initial displacement $x_0/\lambda = -2$. The discrepancies between the 'Helmholtz' and the 'Schrödinger' fields are illustrated on the right hand side by means of differences in the position distribution: they build up from zero, being relatively small near the turning points of the Schrödinger wavepacket, where the transverse is minimal, but increasing with every oscillation.

If the total interaction time is only a fraction of τ_c adding the first few terms of the above series expansion to the Schrödinger solution yields an excellent approximation of te exact Helmholtz field; this is demonstrated in Fig.2 and Fig.3, where the real part of

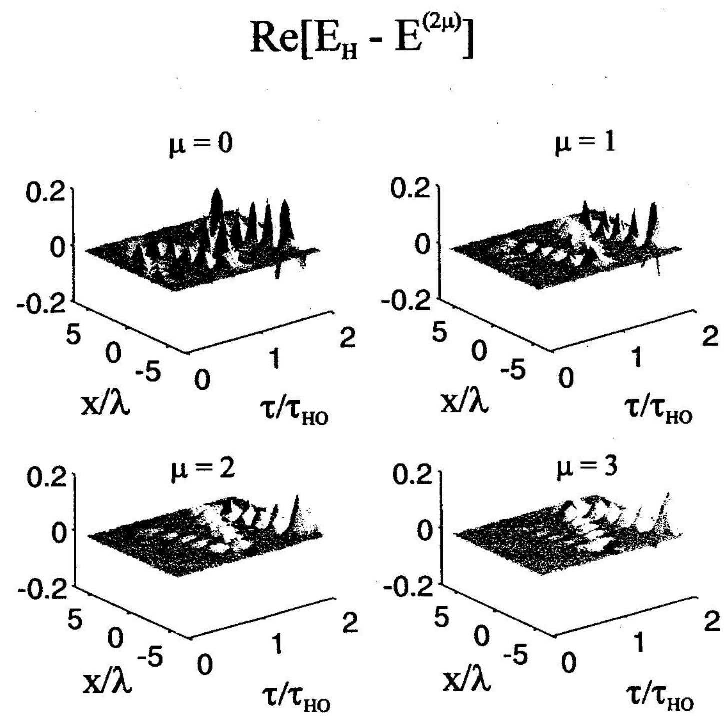

Fig.2. Including the 'optical corrections' up to order μ. Parameters as in Fig.1.

the difference of the Schrödinger wavepacket plus corrections *up to* order μ are shown for $\tau_{final}/\tau_c = 0.28$ and $\tau_{final}/\tau_c = 0.01$, respectively: including higher order corrections the differences are seen to be substantially smaller in magnitude and to occur at later times. Note that there is no significant improvement between $\mu = 2$ and $\mu = 3$ for large times τ.

In Fig.3 the initial displacement is chosen closer to the bottom of the potential $x_0/\lambda = -1$, making the initial wavepacket more 'paraxial' than in the example of Fig.1 and Fig.2. In other words: τ_c is larger now (and thus $\tau/\tau_c = 0.01$) due to the dependence on the eigenvalue E_{n_0} of maximal overlap (which is smaller for a coherent state with smaller displacement).

After having tested the general theory in simple examples, the logical next step is to proceed to more challenging and physically more interesting problems, involving for instance the true vector character of the electromagnetic field: if the three spatial components do not decouple, one can no longer associate one single optical Schrödinger equation with the paraxial wavepacket. Another interesting system to apply our theory to is the tunneling in a double-well potential, which can be viewed as a model for an optical fiber coupler for a paraxial light beam initially confined to one 'fiber', i.e. to one well.

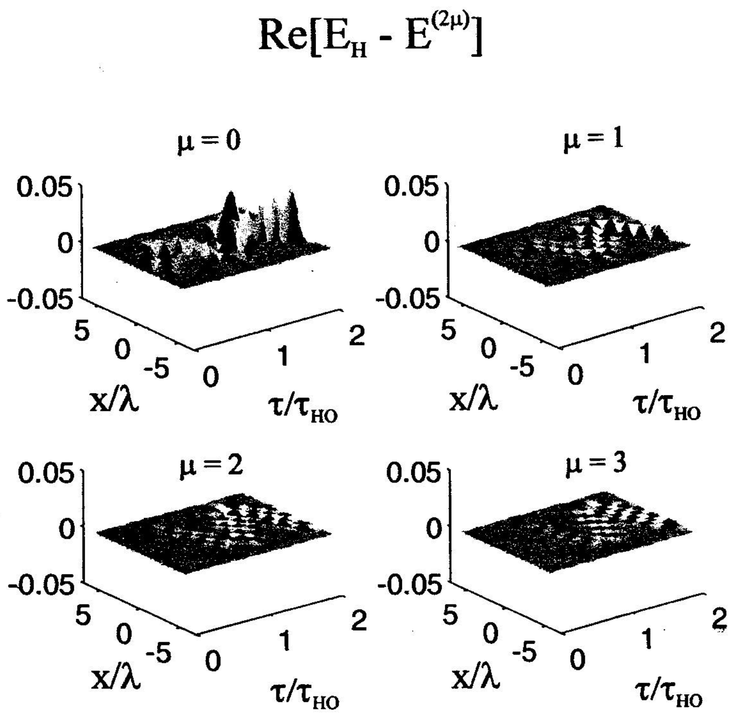

Fig.3. Same as Fig.2, except for a smaller initial displacement $x_0/\lambda = -1$ leading to a more paraxial beam with considerably less differences between the two solutions accumulating in the same interaction time τ_{final}.

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